Siesta Nossi Update

P. Bordat, O. Coulaud, V. Lebris & R. Brown
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1 Non fully periodic Poisson Solver

The following options provide a new Poisson solver for non periodic systems. This method is based on a mutigrid solver from the HYPRE library. We solve the following Poisson problem

$$\Delta V(\vec{r}) = -\frac{4\pi}{\epsilon_0}\rho(\vec{r})$$

with Dirichlet conditions.

Dirichlet conditions are calculated by harmonic expansion of the potential on the surface of the siesta grid. The potential is given by

$$V_p(x) = \sum_{l=0}^{MG.OrderMultipole} \sum_{m=-l}^{l} \frac{(-1)^m}{\|x\|^{l+1}} M_l^m \widetilde{Y}_l^m(\theta,\phi)$$

with $x = (\|x\|, \theta, \phi)$ and, $y = (\|y\|, \theta', \phi')$ and

$$M_l^m = \int_{\mathbb{R}^3} \rho(y)\|y\|^l \widetilde{Y}_l^{-m}(\theta',\phi') \quad ,$$

where the $\widetilde{Y}_l^m$ are spherical harmonic, see INRIA report RR-8221 (2013) (http://fr.arxiv.org/abs/1302.4617).

The parameters of the method are the following

MG.UseMG (*logical*): Specifies use of the multigrid solver for Poisson's equation with Dirichlet conditions.

Default value: `.false.`

MG.SetMGPoints (*logical*): Set the number of points in X, Y and Z explicitly rather than using the built in algorithm which chooses the optimal numbers of points consistent with Mesh cutoff keyword. Deviation from optimal values may degrade performance. If this keyword is set *true*, also specify the numbers of points in each direction with the keywords **MG.NX**, **MG.NY**, **MG.NZ**.

Default value: `.false.`

MG.BCY (*logical*): Specifies periodic boundary conditions in Y.

Default value: `.false.`

MG.BCZ (*logical*): Specifies periodic boundary conditions in Z.
Default value: `.false.`

MG.OrderMultipole (*integer*): The degree of the harmonic explassion used to construct the boundary conditions.
Default value: `4`

MG.Order (*integer*): The order of the finite difference discretisation scheme. Two values are available: 2 implies the 7-point second order stencil and 4 a compact, 16-point fourth order solver.
Default value: `4`

MG.Solver (*integer*): Type of the solver. If 0 PFMG is applied, a semicoarsening multigrid solver that uses pointwise relaxation. If 1 a preconditioned conjugate gradients (PCG) are used. See also the **MG.Precond** and **MG.PrecondIter** options.
Default value: `0`

MG.Verbose (*integer*): If non-zero, each call of the Poissons solver prints the number of iterations to reach convergence and the final residual.
Default value: `0`

MG.Tolerance (*real*): The threshold defining convergence.
Default value: `0.001`

MG.MaxIter (*integer*): The maximum number of iteration to reac the convergence.
Default value: `40`

Advanced options

MG.Precond (*integer*):

Default value: `1`

MG.PrecondIter (*integer*): Maximal number for the preconditionner solver.

Default value: `3`

MG.PreRelaxSteps (*integer*):

Default value: `2`

MG.PostRelaxSteps (*integer*):

Default value: `2`